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A New Approach for Finding All Zeros for Systems of Nonlinear Functions

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Abstract—A new concept in calculation techniques for finding all the zeros for a system of equations of nonlinear functions arising in various applications is presented. The concept is based on the following steps. First, the corresponding system of algebraic equations is created as a homomorphical model for an initial system of nonlinear functions. Second, this system is transformed to a Groebner basis. Third, the algebraic equations are solved by means of the original spectral method using constructing a system of spectral problems for rectangular pencils of matrices. In the paper, the computational symbolic-numerical procedure for this approach is described. The results of calculations based on this technique are presented for an application in theoretical analysis of the properties of the impurity-helium metastable phase under super-low temperatures.

Keywords—Nonlinear functions, Algebraic model, Groebner basis, Spectral method, Symbolic-numerical approach, Impurity-helium meta-stable phase.

1. INTRODUCTION

Mathematical modeling, computer simulation, and virtual prototyping in scientific research and various industrial technologies and processing operations often requires the calculation of all the zeros for a system of nonlinear function's equations (SNFE). In many practical cases, when these functions are algebraic, one can get all solutions using global methods for solving nonlinear algebraic equations [1–4]. However, when these functions are not algebraic, the problem to find all zeros for the SNFE is often much more difficult. For example, Gordon *et al.* [5] have reported on severe difficulties in solving SNFE arising in the theoretical attempt to realize the cluster approach in describing quantum-mechanical helium atoms behavior at low temperature. This paper discusses a new concept that can overcome such obstacles and can allow for finding all the zeros for SNFE in the case when it is ill-conditioned or has some other computational difficulties.

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2. PROCEDURE FOR CALCULATION

Without loss generality, here we will consider the following class of SNFE that consists of the function and its first partial derivatives on each variable:

$$\begin{aligned} &F(x,y,\dots) = \sum_i^k a_i \frac{M_i^{p_i}(x,y,\dots)}{N_i^{q_i}(x,y,\dots)} = 0; \\ &F_x(x,y,\dots) = 0; \\ &F_y(x,y,\dots) = 0; \\ &\qquad\vdots \end{aligned} \tag{1}$$

It is necessary to make a few remarks concerning the SNFE under consideration. First, all members of the SNFE above belong to the same class of polynomial functions. Second, the number of equations in the initial SNFE does not have to be less than the number of unknowns. And third, if each member of the SNFE is reduced to the common denominator for solving the system of nonlinear algebraic equations (SNAE) that are thus obtained, it may lead to the loss of the part of the common solutions. To avoid the last obstacle, we suggest the construction of an algebraic model for the SNFE that could be solved by standard methods for solving SNAE. For that purpose, new variables are defined as follows:

$$u_i = \frac{1}{N_i(x,y,\dots)}, \quad v_i = M_i(x,y,\dots), \qquad i = 1,\dots,k. \tag{2}$$

Then system (1) may be rewritten as

$$\begin{aligned} &F(u,v,\dots) = \sum_i^k a_i u_i^{q_i} v_i^{p_i} = 0; \\ &F_x(u,v,\dots) = 0; \\ &F_y(u,v,\dots) = 0; \\ &\qquad\vdots \end{aligned} \tag{3}$$

System (3) so obtained is an algebraic model for the SNFE in the form of a SNAE. Then system (3) can be viewed as a system of polynomials

$$F : f_j(u_i, v_i), \qquad j = 1,\dots,m. \tag{4}$$

As is known, either symbolic methods or numeric ones [6] can be used for finding all solutions of (4). Recently, the idea to use an approach including mixed symbolic-numerical calculations appeals to researchers [7]. We decided to apply this idea in solving the above problem. Following [1], system (4) can be transformed into a Groebner basis

$$G : g_l(u_i, v_i), \qquad l = 1,\dots,n. \tag{5}$$

It is important to note that for some problems the number of polynomials in system (5) may be different from that of in system (4). The most interesting case for the problem under solution is when the number of polynomials is not less than in system (4). Hence, system (5) has the same solutions as the previous one. As a result, one obtains the solution of system (4) in a symbolic form. However, in practice the initial data for calculations often come from experiments and are in numerical form. This makes it necessary to get the solution of the task in the same form.

For this purpose we have developed our own direct method for solving SNAE in a floating point arithmetic on the basis of spectral decomposition of singular pencils of matrices. For the first time the idea of the method was described in 1978 by the Russian mathematician Kublanovskaya [8]. At that time, no way could be found its practical application because no effective computing algorithm existed for determination of the Kronecker canonical forms (KCF) for rectangular pencils. In the 1980s, Van Dooren, a Dutch researcher, proved a series of theorems connected to the spectral structure of matrix pencils and demonstrated the capability of reducing a singular matrix pencil to a quasi-triangular polynomial form containing two blocks [9]. The first of these unites all infinite eigenvalues and the right-hand polynomial indices, and the second one unites the finite eigenvalues and left-hand polynomial indices. It is necessary to emphasize that this direct method for solving SNAE, based on Kublanovskaya's approach, is a global one. It does not use the information from the Jacobean for the set of equations being solved and does not require a linearization that is typical for such iterative methods as, for instance, the Newton method. It is based on a property of an algebraic structure of a null space of the SNAE. It allows for the construction of a system of spectral problems for rectangular pencils of matrices. In this way, the solutions of SNAE are determined as eigenvalues of regular blocks of matrix pencils [10]. A practical algorithm for the solution of SNAE based on this approach and its application to the solution of real physical problems has been demonstrated in several papers [2,3].

After obtaining the solution for system (4) by means of the method cited above, one has to return to solving the SNFE using expression (2):

$$\begin{aligned} N_i(x,y,\dots) &= \frac{1}{u_i}, \\ M_i(x,y,\dots) &= v_i, \qquad i = 1,\dots,k. \end{aligned} \tag{6}$$

System (6) presents by itself a system of nonlinear algebraic equations (SNAE). It means that by solving the two sets of equations (3) and (6), one can get the solution for the SNFE that corresponds to the algebraic model (3) that has been developed.

The algebraic model built on the basis of the procedure described above will possess only part of the properties of the initial SNFE. So here and below we will define it as a homomorphic algebraic model (HAM) of the initial problem.

In the next section, we will describe a computational example of how to use the approach developed for solving a specific system of nonlinear functions.

3. COMPUTATIONAL EXAMPLE

In the theoretical model by Gordon *et al.* [5], the interaction between the impurity and the helium atom was a Van der Waals one and decreased as R^{-6} with the growth of the distance, R, between the impurity and the atom. One of the models considered leads to the following form of the SNFE:

$$\begin{aligned} F(x,y) &: \frac{1}{(y-6x)^6} - \frac{1}{(y-3x)^3} + E + \frac{b}{x}; \\ F_y(x,y) &: \frac{2}{(y-6x)^7} - \frac{1}{(y-3x)^4}. \end{aligned} \tag{7}$$

This set of nonlinear functions has been created from algebraic polynomials by means of nonlinear operations. Only one nonalgebraic operation, namely division, was applied in this case. The SNAE can be formed as the HAM for the initial SNFE as follows:

$$\begin{aligned} u^6 - v^3 + q &= 0; \\ 2u^7 - v^4 &= 0; \end{aligned} \tag{8}$$

where

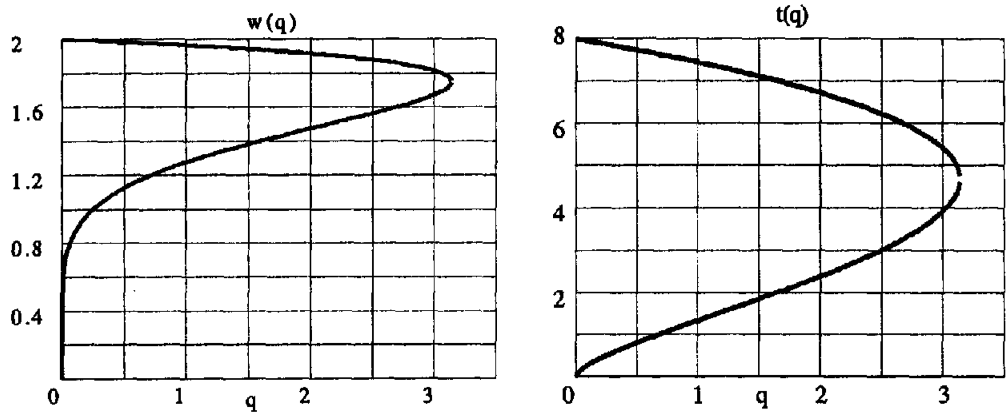
$$\begin{aligned} q &= E + bx > 0, \qquad (E > 0, b > 0, x > 0); \\ u &= \frac{1}{(y-6x)}; \\ v &= \frac{1}{(y-3x)}. \end{aligned}$$

Introducing new variables $w = u/v$ and $t = u^3$, the following SNAE of two equations is obtained:

$$\begin{aligned} t^2 - w^3 t + q &= 0; \\ 2t - w^4 &= 0. \end{aligned} \tag{9}$$

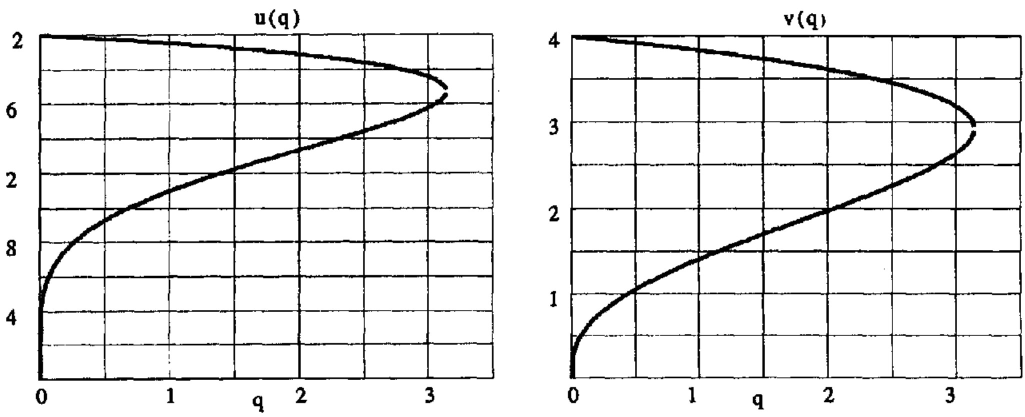
A Groebner basis for system (9) for the case when q is a parameter was created by the standard procedure in the software MAPLE V [11] and is written as

$$Gtw = \begin{cases} -2t + w^4; \\ -t^2 - w^3 t - q; \\ -2t^2 + wt^2 + wq; \\ w^3 q + 2w^2 q + t^3 - 8t^2 + 4wq + tq. \end{cases} \tag{10}$$



(a) (b)

Figure 1. Variables w (a) and t (b) vs. parameter q.



(a) (b)

Figure 2. Variables u (a) and v (b) vs. parameter q.

This system of polynomials in a Groebner basis is solved by MATLAB Toolbox SNAE [12] that provides the following dependencies for the variables w and t versus the parameter q. These dependencies are shown graphically in Figures 1a and 1b. Then using the substitutions introduced above, the curves shown in Figures 2a and 2b are obtained for the variables u and v. At the next stage of the calculation procedure, the solutions for the initial variables x and y are determined by solving the following system:

$$\begin{bmatrix} 1 & -6 \\ 1 & -3 \end{bmatrix} \begin{bmatrix} y \\ x \end{bmatrix} = \begin{bmatrix} \dfrac{1}{u} \\ \dfrac{1}{v} \end{bmatrix}. \tag{11}$$

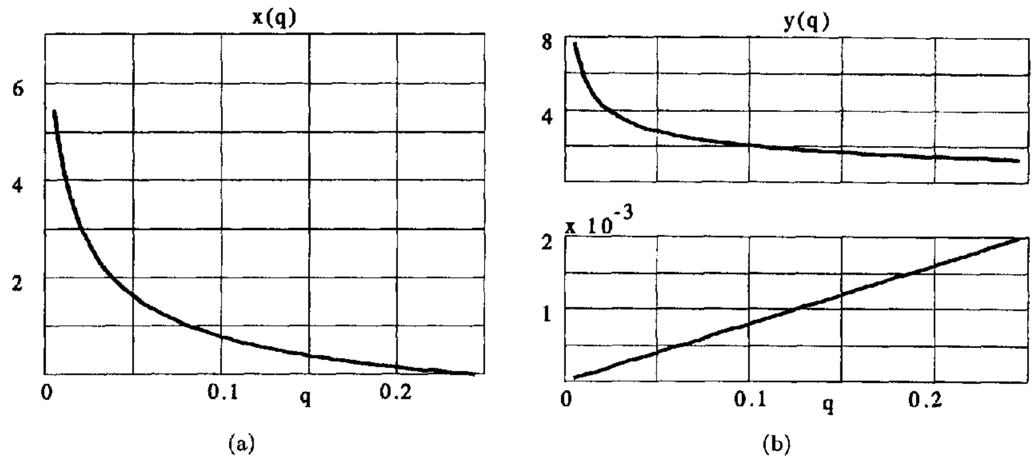


Figure 3. Variables x (a) and y (b) vs. parameter q.

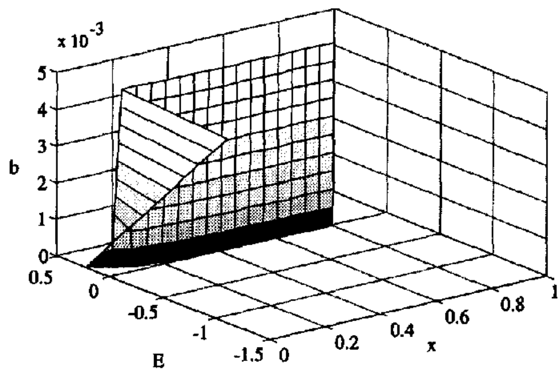


Figure 4. All zeros for the initial SNFE vs. parameters E and b.

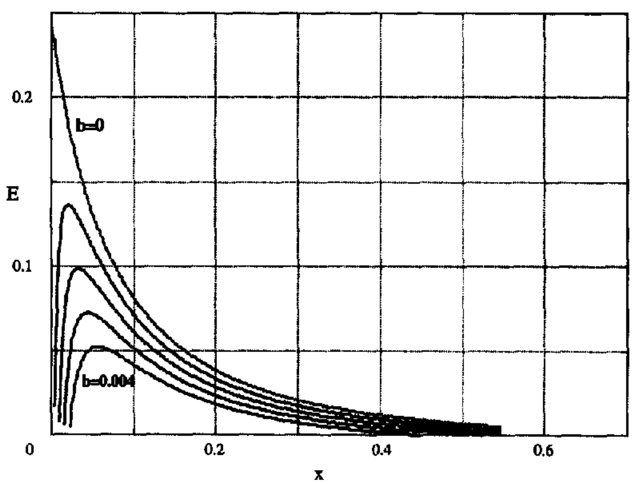


Figure 5. The solutions x vs. E for various values of the parameter b.

It should be noted that the approach suggested also allows system (11) to be considered in the case that they are nonlinear algebraic equations. Then taking into account the condition that x and y are greater than zero, one can get the dependencies $x(q)$ and $y(q)$ shown in Figures 3a and 3b. Finally, the results of calculating all zeros for the initial SNFE are presented in Figure 4. The results obtained are demonstrated in the coordinates (x, E, b), where E and b are the parameters of the initial SNFE. The accuracy of the solution obtained was $2.7 \cdot 10^{12}$. The projection of the 3D surface in Figure 4 to the (E, x)-plane for $0 \leq b \leq 4e-3$ with an increment of $1e-3$ is represented in Figure 5.

4. CONCLUSIONS

A new concept for finding all solutions for systems of nonlinear functions is suggested. It is comprised of the following steps. First, a system of nonlinear algebraic equations transformed from the nonlinear functions is created as a homomorphic model for the initial problem. Second, a Groebner basis is constructed by using standard computing software. Third, a new system of nonlinear algebraic equations is solving by means of the direct method developed by the authors on the basis of spectral decomposition of singular pencils. Fourth, the results obtained are analyzed from the point of view corresponding to the initial problem. The computational example chosen from theoretical research for the problem of metastable impurity-helium in the solid phase under super-low temperature confirms the ability of the approach suggested to get all zeros for ill-conditioned problems.

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